T-1
Mechanics of Materials & Equation-of-State

# Modeling Metallic Microstructure Using Moving Finite Elements

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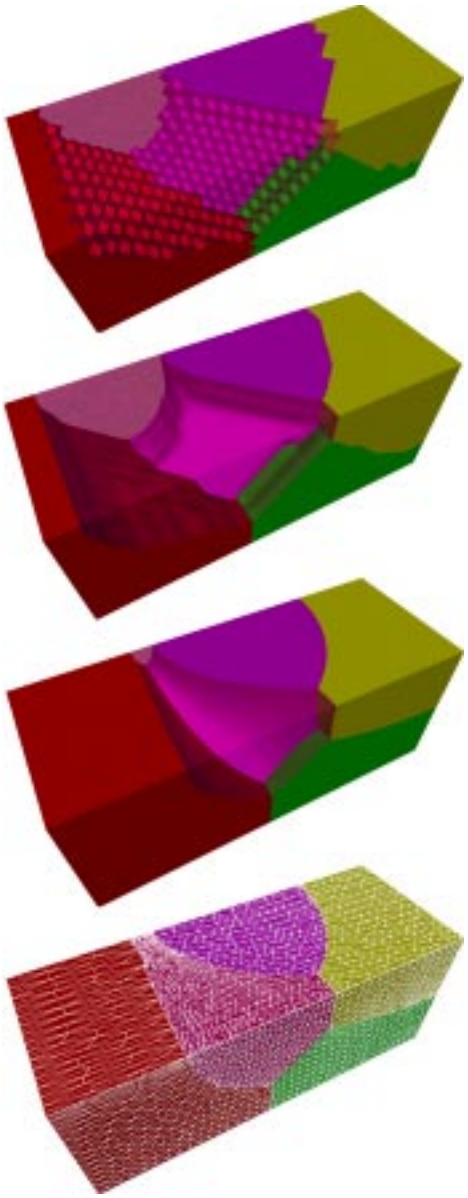
To attack the general problem of evolution of metallic grain microstructure in 3D, we employ two different methods: using Monte Carlo (MC) techniques to anneal an effective discrete model on a fixed lattice [1], and using Gradient Weighted Moving Finite Elements (GWMFE) to evolve grain boundaries by mean curvature (local velocity proportional to the local curvature)–the simplest continuum model for grain evolution [2, 3]. These two models reduce to each other in the appropriate limits. MC has the advantage of computational and algorithmic simplicity while GWMFE is more easily adaptable to including coupled transport fields such as vacancies and impurities, and other geometrical and physical complexities occurring in the simulation of interconnect-via interactions as related to electromigration reliability of submicron integrated circuits. Crosscomparisons of the two calculational techniques will produce the best synthesis of accurate physical models and computational speed. We also compare to other methods, such as 2D front-tracking [3].



In the finite element approach, we represent the metallic grains on an unstructured tetrahedral mesh, generated using the LANL X3D grid code. We use an implicit implementation of the GWMFE method to move the grain surface (interface) triangles. Although volumes are deformed by the moving grid, the computational complexity of the method is only 2D, not 3D, because GWMFE moves triangles, not tetrahedra [2]. Figure 1a shows an intermediate MC evolved microstructure, with the average grain size approximately half the width, which we used as input to GWMFE. After a few GWMFE time steps, the initially jagged interfaces between the grains (a consequence of the fixed fcc lattice used in the MC simulation) have begun to smooth out under the action of mean curvature motion (Figure 1b). In Figure 1c, GWMFE has evolved the microstructure to a completely smooth state. Visible in the interior, due to one of the foreground grains being made "semitransparent," are "triple lines," where three grains meet at 120° angles, and "tetrahedral points" where four materials meet. On the surface

***Figure 1: GWMFE evolved microstructure as a function of dimensionless time (surface tension of order 1 and spatial dimensions of order 1): (a) t = 0: MC model evolved microstructure used as input; (b) t = 0.1: GWMFE has smoothed the initially jagged interfaces. There is otherwise no significant grain boundary motion; (c) t = 30: The smooth boundaries allow use of large time steps in the implicit adaptive GWMFE scheme; and (d) Underlying surface grid of triangles at the same time as in (c). (Volume tetrahedra are obscured.) Topological change is necessary at this point.***

of the geometry, we see that the boundary constraint leads to several triple points (analogous to 2D simulations). All interface angles agree with predictions for mean-curvature motion. However, the underlying grid (Figure 1d) composed of interface triangles is becoming distorted, and must be refined in some areas and derefined in other areas. Although the X3D code can accomplish the necessary topological changes in a semiautomated manner at this time, we are currently completing development of a fully-automated topological analyzer called "Graph Massage" which will seamlessly accomplish the necessary topological changes for the simulation to continue while preserving grain interfaces. High-level routines detect major topological "events" (such as the collapse of an entire grain, which is then simulated correctly by restricting mesh connectivity changes to only those that sufficiently preserve material volumes). We next plan to investigate grain boundary evolution under isotropic thermal strain starting from initially randomly oriented grains.

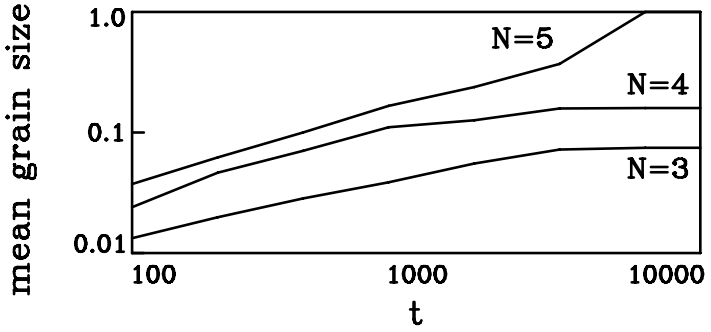



***Figure 2: Mean grain size normalized to the total volume as function of time and number of neighbors N from Monte Carlo evolution of the Potts model [1] on an unstructured grid generated by the LANL X3D grid code. Note growth stagnates for N<5.***

Having the ability to use MC grain evolution on X3D generated geometries and meshes, such as those of the confined geometry of an Al interconnect on a semiconductor chip, makes it an extremely useful tool to generate realistic input for the GWMFE code. The MC code evolves an initial microstructure of randomly-oriented grains on a fixed lattice using a discrete effective classical spin model originally developed to model magnetic domains (Potts model) [1]. For the first few time steps, MC scales with the number of volume points. Activity binning and N-fold or cluster flip MC techniques allow significant speedups in the time evolution [1]. (Incorporation of volume information may reduce these speedups.) On a regular fcc lattice discreteness trapping is known not to be a problem [1]. However, on the unstructured grids resulting from the LANL X3D code, we see from Figure 2 that 5th neighbor interactions are needed in order to get normal grain growth without pinning at finite grain size. We are investigating how various algorithms for treating further neighbors effect these MC grain growth statistics.

To add the capability of correctly modeling grain boundary evolution in the environment of time-dependent stress and strain due to unsteady and spatially nonuniform temperature and impurity gradients, it will be necessary to couple the GWMFE code to a truly 3D physics code. Currently under development for this purpose is the Arbitrary Lagrangian Finite Element (ALFE) code which is a fully-implicit Galerkin Finite Element method for tracking the evolution of fully-coupled systems of partial differential equations. The code under development will use the latest "matrix-free" iterative methods, and thus will be highly parallelizable. The fully-implicit adaptive time-stepping scheme used will allow for efficient resolution of phenomena at various time-scales, while access to the X3D adaptive grid refinement capabilities will allow ALFE to track phenomena at various spatial scales as well. Finally, we note that ALFE is an "Arbitrary Lagrangian" code, which means it has the capability of correctly tracking the evolution of phenomena in an arbi-trary, spatially and temporally nonuniform, coordinate system. This is crucial for the grain-growth simulation, where volume tetrahedral movement is "slaved" to the interface triangle movement computed by GWMFE.

We are also currently evaluating a 3D electromigration simulation code from Motorola which will take as input the microstructure from Figure 1 and predict electromigration reliability for the interconnect being simulated. These studies will establish whether the additional overhead of a fully 3D model is justified, or if 2D simulations [3] adequately describe the evolved microstructure. We expect that 3D models will be important in intrinsically nonplanar geometries, such as vias.

[1] E. A. Holm, Ph.D. Thesis, University of Michigan, 1992, unpublished.
[2] Andrew Kuprat, in the Proceedings of the Fifth International Conference on Numerical Grid Generation in Computational Fluid Dynamics and Related Fields, Mississippi State University, Mississippi, 1-5 April, 1996.
[3] H. J. Frost and C. V. Thompson, *J. Elec. Mater.* **17,** 447 (1988).

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